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U.S. Army Research Laboratory Gun Tube Erosion Code (ATEC) User's Guide

by Paul J. Conroy

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1. Introduction

The U.S. Army Research Laboratory Gun Tube Erosion Code (ATEC) is the culmination of effort by the U.S. Army Research Laboratory (ARL) to identify the thermochemical components to gun tube erosion. The inclusion of chemistry was originally conceived due to discrepancies of experimentally fired propellants to the previous correlations. The historical correlations were based solely on the propellant's adiabatic flame temperature and did not take into account the possible chemistry. To address this deficiency, ARL embarked on a project to include chemistry in a model which would enable the prediction of erosion from basic principles without requiring too much information prior to the actual system investigation. The model needed to be system independent with enough basic physics such that it would function for most guns or gun-like systems irrespective of caliber. To this end, a modular gun tube erosion code was developed. Technical details of the code, as well as results, have been previously reported by Conroy et al. [1-6] and Weinacht and Conroy [7].

The following physical phenomena are included in the model:

- Convective heat transfer to the surface through convection coefficients,
- Subsurface heat conduction with variable physical properties for gun steel,
- Multicomponent species mass transport to the surface, independent of heat transport,
- User-specified finite rate surface reactions,
- Subsurface, diffusion limited, equilibrium reactions with user-specified reactants and products,
- User-specified coating materials,
- Coating stress/crack distribution calculation,
- Erosion at the base of cracks in surface coatings, and
- Uncoated surface erosion.

This report documents the ATEC user input as well as output from the code. Instructions for developing an input deck are explicitly provided in the following sections. Files required to operate the code include a user-generated input deck, "erod.in", an output file "htemp.out" from XKTC [8], the NASA Lewis library "library.in" [9], and a species temporal file, "species.out", from a coupled interior ballistic-equilibrium thermodynamic code.

Example input decks are provided in Appendices A and B. An example of the "species.out" file is given in Appendix C. The ATEC code has been applied to

the 25-mm Bushmaster cannon, Navy MK45 5-in cannons, the 120-mm M256 tank cannon, as well as various vented fixtures, and has performed well in representing the physics occurring at the surface.

2. General Computer Model Description

Figure 1 represents what occurs beneath the coating near a crack. What is evidenced is that a jet of combustion gases washes through the crack subsequently reacting and eroding the substrate material leaving a pit with horizontal extensions near the interface. Many species of materials in the eroded region have been identified and include sulfur, oxygen, and talc from the propellant additives [10, 11]. An interesting observation is that sulfur penetrates deep into the eroded pits. Sulfur comes from the black powder ignitors and potassium sulfide flash suppressants used in the charges.

Figure 2 is a cartoon of the numerical simulation of erosion at the bottom of a radial crack. It is important to realize that crack orientation is critical, for if the crack is longitudinal, it would enable propellant product gases to wash directly in and out with tremendous amounts of heat transfer and the possibility for surface reaction, in comparison to a radial crack which would rely more on recirculation and diffusion of gases to the interface.

Figure 3 shows the interconnectivity of the codes for an erosion calculation. The interior ballistics is modeled yielding the thermochemistry of the propellant products for further transport to the surface, as well as supplying gas state and velocity variables for convection heat transfer. The erosion code itself has an extensive input deck, the description of which is the purpose of this report.

3. Required U.S. Army Research Laboratory Gun Tube Erosion Code (ATEC) Input Data Files

Table 1 provides a guide to all input/output files for the ATEC code. The following are required input files:

(1) A mixed free format and formatted input data deck specific to ATEC called "erod.in". This input deck is described in detail in this guide.

(2) A data file from the XKTC 1-D NOVA code entitled "htemp.out".

(3) A data file entitled "species.out". An example of this file is supplied in this report. It can be generated by any number of coupled interior ballistic and thermodynamic equilibrium codes such as XKTC with NASA Lewis.

(4) The NASA Lewis species thermochemistry library. This provides the thermochemistry for both the equilibrium and finite rate kinetics calculations.

Note: Lower case should be used for input file names.

The following is the format required of the file "species.out".

The first line contains the header "-Time_(ms)" followed by the names of the up to top 25 resultant species from the equilibrium calculation entered in the following format where the names are entered as "6a1" in standard NASA Lewis format.

```
      READ(30,850) ((ZLABEL(II,JJ),JJ=1,6 ), II=1,SPNDIM2)
850   FORMAT( ' -Time_(ms)', 25(', --',6a1,'-') )
```

Note: The species should be in descending order from highest initial molar concentration to the lowest, from the second to the leftmost column to the last column to the right.

Inclusion of the top 25 species should suffice for calculations purposes. The lines following the first line of the input file "species.out" contain the time history of each species concentration with the first column tracking time in milliseconds and the following columns containing the species concentration in mole fractions in the format presented in the following read statement:

```
      READ(30,860, END=2000)(VAR(KT1,KN1,NV),NV=1,SPNDIM2+1)
860   FORMAT( 1X,F10.4, 25(',',1PE10.3) )
```

An example of a "species.out" file is provided in Appendix C.

4. ATEC Input Deck Generation Guide

0.1 Examine the htemp.out output file from XKTC.

Determine initial grid spacing (in).

Determine initial temperature (R).

Determine initial chamber length (in).

Determine final length of the tube from the last time step (in).

1.1 Enter the initial temperature from the htemp.out file (R).

1.2 Enter the initial pressure from the htemp.out file (R).

1.3 Enter the initial velocity from the htemp.out file (in/s).

2.1 If there is an inner surface coating layer enter thickness (in).

2.2 Enter total time of each firing (ms).

2.3 Usually the chamber augmentation factor is 0.1 (-).

2.4 Enter the chamber length (in).

2.5 Enter the tube length from the last time step of htemp.out file (in).

2.6 Enter the number of axial grid points (<100).

This is not a trivial task!

The INITIAL (t=0) grid spacing from the htemp.out file MUST BE GREATER than the erosion grid spacing. If you wish to examine the entire barrel length, you may have to accomplish this in more than one calculation as the code currently accepts 100 axial points, where NOVA usually has 50 or more distributed over about a 40-in chamber, for example.

2.7 Determine the computational region desired.

Make sure the length of the computational space doesn't expand the grid spacing beyond the initial htemp.out grid spacing.

Enter the calculation starting position (in).

This must be within the specified tube geometry.

2.8 Enter the calculation ending position (in).

This must be within the specified tube geometry.

2.9 If 2-D LP chamber calculation, enter a one to trip flag (LP option).

(Not currently implemented in erosion code, i.e., must be zero.)

2.10 If 2-D LP chamber calculation, enter the initial piston offset (in) (LP option). **(Not currently implemented in erosion code, i.e., must be zero.)**

2.11 If IMC cooling is desired, enter 1 (this is a flag for an extra card).

(Not currently implemented in erosion code, i.e., must be zero.)

2.12 If the outside surface is insulated, enter 1.

(Not currently implemented in erosion code, i.e., must be zero.)

2.13 If blowby is desired, enter 1 (this is a flag for an extra card).

(Not currently implemented in erosion code, i.e., must be zero.)

2.14 Enter the amount by which you want to multiply the internal convective heat transfer coefficient. If no multiplication is desired, enter 1.D0 or 0.0 (both produce the nominal result).

C1.1 This is conditional on the heat transfer coefficient augmentation in 2.14. If a negative value is entered, then a roughness calculation is performed based on defects on tube surface and Moody chart. Enter smooth deformation limit (m).

C1.2 Enter rough deformation limit (m).

3.1 Enter the number of axial locations to be specified (-).

3.2-9 Enter up to eight axial locations (in).

4.1-8 Enter up to eight corresponding outer diameters (in).

5.1-8 Enter up to eight corresponding inner diameters (in).

Breech is zero. Calculation occurs in specified computational space.

6.1 Enter the number of probe locations, up to eight axial locations (-).

6.2-9 Enter up to eight axial locations (in).

7.1-8 Enter up to eight corresponding probe locations in the tube (in) .

Note: The probe depth is only printed to two decimal places, so don't be surprised when you ask for a probe at 0.005 inches and it comes back as 0.01 inches. It is just an artifact of the print format. The probe depth is from the bore surface into the tube!

8.1 Enter "1" to activate only the equilibrium surface chemistry.

Enter "2" to activate both the subsurface equilibrium chemistry and finite rate surface chemistry

Enter zero if you wish to bypass the chemistry (-).

8.2 Enter the freeze-out temperature (K), i.e., temperature at which the transport/surface chemistry routine is not called.

8.3 Enter density of the base wall material (kg/m^3).

8.4 Enter temperature at which the base wall material begins to melt (K).

8.5 Enter specified outer barrel heat transfer coefficient ($W/m^2/K$).

8.6 Enter ambient outer air temperature (K).

8.7 Enter the computational coordinate spacing (-) usually "1".

8.8 Enter the latent heat of fusion for the material (J/kg).

8.9 Enter "0" if the system is planer or "1" if the system is axisymetric.

8.10 Wall temperature calculation flag (-).

Molecular weighting function between gas and solid.

Wall temperature.

Conditional Card (if Chrome > 0).

C2.1 Number of radial points considered in coating for calculation (-).

C2.2 Number of radial points considered in base material for calculation (-).

C2.3 Enter the freeze-out temperature of surface material (K), i.e., temperature at which the chemistry routine is not called.

C2.4 Enter density of the coating material (kg/m^3).

C2.5 Enter temperature at which the coating material begins to melt (K).

C2.6 Enter the computational coordinate spacing (-) usually "1".

C2.7 Enter the latent heat of fusion for the coating material (J/kg).

C2.8 Stress flag (0)-no stress calculation (1)-stress calculation (-).

Conditional Card (if Chrome > 0).

C3.1 Enter the Young's modulus of the coating material (Pa).

C3.2 Enter the Coefficient of Thermal Expansion of the Coating (1/K).

C3.3 Enter the Poisson's Ratio Coating (-).

C3.4 Enter the ultimate Strength of Coating (Pa).

C3.5 Enter the Young's Modulus Base (Pa).

C3.6 Enter the coefficient of Thermal Expansion Base (1/K).

C3.7 Enter the Poisson's ratio of the base material (-).

Conditional Card (if Chrome > 0).

C4.1 Enter crack width (m).

C4.2 Enter crack distribution limit (m).

10.1 Enter the number of shots to fire.

(Not implemented in this version of Erosion Code, i.e., must be 1).

10.2 Enter print frequency during htemp.out file period (-). Choosing the computational time interval (implicit) (usually about 0.1 ms) enables the print frequency to be entered, i.e., print every x time steps.

10.3 Enter print frequency after htemp.out file period (-).

10.4 If restarting, enter the number of the last round fired before restart, else enter a zero.

(Not implemented in this version of Erosion Code, i.e., must be 0).

11.1–11.17 Control the files to be printed.

(o = false), (1 = true), (2 =>single shot = burst)

1. 0 = K, 1 = R (units Rankine or Kelvin)
2. 0 = as computed, 1 = temperature rise
3. Screen output IOUT(1)
4. Single shot probe temperature IOUT(2)
5. Single shot inside surface temperature IOUT(3)
6. Single shot outside surface temperature IOUT(4)
7. Burst fire probe temperature IOUT(5)
8. Burst fire inside surface temperature IOUT(6)
9. Burst fire outside surface temperature IOUT(7)
10. Heat transfer coefficient IOUT(8)
11. Effective gas temperature history IOUT(9)
12. Single shot graphic output file (for IBGRAF movies) IOUT(10)
13. Burst fire graphic output file (for IBGRAF movies) IOUT(11)
14. Boundary condition graphic output (for IBGRAF movies) IOUT(12)
15. Bore surface heat flux output (single shot-1, burst-2) IOUT(13)
16. Bore surface regression rate (single shot-1, burst-2) IOUT(14)
17. Bore surface regression (single shot-1, burst-2) IOUT(15)
18. Bore surface concentrations IOUT(16)
19. Bore core flow concentrations IOUT(17)
20. Shear stress azmuthal at interface IOUT(18)
21. Shear stress axial at interface IOUT(19)

(Note: Screen output is for PC applications only and is not supported.)

12.1 Variable 4340 conductivity and diffusivity flag 1-use internal functions, 0-use input values.

12.2 Barrel conductivity (W/m/K) (Necessary even if 12.1 is 1.)

12.3 Barrel diffusivity (m^2/s) (Necessary even if 12.1 is 1.)

12.4 Liner conductivity (W/m/K) Necessary even if 12.1 is 1.)

12.5 Liner diffusivity (m^2/s) (Necessary even if 12.1 is 1.)

(A selection of this information is provided in Appendix A.)

13.1 Enter the flag number = "42" upon which the equilibrium chemistry read section is keyed (if you use the kinetics, you must include all species from the kinetics section in the equilibrium section in order to load the thermo-chemical arrays.)

14.1 Enter the following phrase with the following format as a key for chemistry read section:

FORMAT(A30,I3): "NUMBER OF REACTANT ELEMENTS = "

15.1 Enter the number of gas phase reactant elements considered (-).

16.1 Enter the following phrase with the following format as a key for chemistry read section:

FORMAT(A30): "CONSIDERED ELEMENTS = "

17.1–17.n Enter the "n" gas phase elements considered in atomic order FORMAT(n(A4))

18.1 Enter the following phrase with the following format as a key for chemistry read section:

FORMAT(A30): "REACTANTS"

Enter reactant information using **FORMAT (5A4,4(A2,F3.0),A1)**

19.1–19.5 Enter the reactant species name (left justified) as it appears in the N-L library.

19.6–19.7 Enter the first element symbol (left justified) and the number of atoms (right justified).

19.12–19.13 Enter the last element symbol (left justified) and the number of atoms (right justified). Leave any extra fields blank.

19.14 Enter the phase as "G", "S", or "L" for gas, solid, or liquid state.

19.15 Enter Critical Pressure PCRIT (Pa).

19.16 Enter Critical Temperature (K).

19.17 Enter SIGMA for Lennard Jones diffusion Å.

19.18 Enter Epsilon over K EPSOK for Lennard Jones diffusion (K).

...

Continue with Card 19's until all gaseous reactants have been entered.

20.1 Enter the following phrase with the following format as a key for chemistry read section:

FORMAT(A30): "PRODUCTS"

...

21.1 Enter the considered products (gaseous, liquid, solidus) in the same manner as the reactants with the same format until all products are entered.

Note: To match internal keyed indices:

The 9th reactant must be C(GR).

The 10th reactant must be FE(A).

The 11th reactant must be FE(C).

The 15th species (#Reactants + #Products) must be FE3C.

Kinetics data input follows

C2 Enter the following phrase with the following format as a key for kinetics read section:

FORMAT(A30): "KINETICS BEGIN REACTION CARDS"

Contingent upon 8.1 = 2.

C.3.1 Enter number of kinetics reactant species (-).

C.3.2 Enter number of kinetic reactions (-).

C.4.1 Enter considered reactant species FORMAT(4(5A4)).

Enter reactant information using FORMAT(A10,7E10.4,I5).

C.5.1 Enter key word "REACTANTS".

C.5.2 Enter forward rate coefficient CF in (cm^3/mole-s) or (cm^6/mole^2-s).

C.5.3 Enter forward rate temperature exponent ETAF (-).

C.5.4 Enter forward rate activation energy EF/k (K).

C.5.2 Enter backward rate coefficient CB in (cm^3/mole-s) or (cm^6 /mole^2-s).

C.5.3 Enter backward rate temperature exponent ETAB (-).

C.5.4 Enter backward rate activation energy EB/k(K).

If backward rates are entered as zero then they are not considered, if they are entered as "-1" then rates are determined from thermodynamic data.

C.5.5 Enter third body flag THIRDBODY (-) (1=T, 0=F).

C.5.6 Enter surface or gas phase reaction flag ICOFU (-)

(0 NORMAL 1 = SURFACE)

Enter reactant and product data using:

FORMAT(5A4,F3.0,4(A2,F3.0),A1,4E10.4)

C.6.1 Enter reactant of first reaction using NASA Lewis library notation (-).

C.6.2 Enter coefficient of first atomic in reactant (-).

C.6.3 Enter first atomic of first reactant (-).

C.6.4 Enter second coefficient of second atomic in reactant (-) blank if non-existent.

C.6.5 Enter second atomic of first reactant (-) blank if non-existent.

C.6.6 Enter third coefficient of third atomic in reactant (-) blank if non-existent.

C.6.7 Enter third atomic of first reactant (-) blank if non-existent.

Enter all reactants as previous.

C.7.1 Enter key word "PRODUCTS".

C.8.1–C.8.7 Enter product data using reactant data guide.

CC.1.1 If reaction is third body, enter key word "EFFICIENCY".

CC.1.2 Enter efficiency for reaction to each kinetic reactant species in the order entered in C.4.1. FORMAT(7(F10.0)).

CC.2.1 If reaction is not a third body reaction, enter key word "KEND".

...

Continue with next reaction card set C.5–CC.2 until reactions are completed.

5. ATEC Card/Variable Definitions

Card 1: Initial State of Bore Gas

TINIT	Initial Gas Temperature (NOVA run, R)
PINIT	Initial Gas Pressure (NOVA run, psi)
UINIT	Initial Gas Velocity (NOVA run, in/s)

Card 2: Flags, Counters, and Grid Layout

CHROME	Thickness of chrome layer (in)

TMAXV	Total time per shot, i.e., from the firing of one shot to the next shot(ms)
XCON	Breech velocity augmentation for singularity point (-)
XCHAMB	Chamber length (in)
ZMAX	Total barrel length (in) = (chamber length + tube length) (in)
NLOC	No. of axial grid points (< 100, keep larger than 25)
ZSTART	Start of distribution of 100 axial points (in)
ZEND	End of distribution of 100 axial points (in)
LP2D	Flag for 2-D LP chamber calculations (-) **This function is NOT IMPLEMENTED, enter 0.**
LPOFFSET	Initial piston offset for 2-D LP chamber calculations (in) **This function is NOT IMPLEMENTED, enter 0.**
IMC	Flag to cause IMC card to be read for forced convection boundary condition for representing integral midwall cooling (-) **This function is NOT IMPLEMENTED, enter 0.**
INSOBC	Flag to trip insulated outer barrel surface (-) **This function is NOT IMPLEMENTED, enter 0.**
LBLOWBY	Flag to cause blowby multiplication factors card to be read (-) **This function is NOT IMPLEMENTED, enter 0.**
AUGMENT	Convective heat transfer multiplication factor 1.0 or user specified value (-)

Conditional Card 1: Roughness Data (if AUGMENT is negative)

ESMOOTH	Smooth deformation limit (Moody Chart) (m)
EROUGH	Rough deformation limit (Moody Chart) (m)

Card 3: Barrel Geometry

NDTZ	No. of axial barrel geometry description locations (up to 8)
ZDB(1-NDTZ)	Axial Location (in)

Card 4: O.D.

DBAR(1-NDTZ)	Barrel O.D. at the location (in)

Card 5: Inner Diameter

DBOR(1-NDTZ)	Barrel I.D. at the location (in)

Card 6: Probe Location Information

NHTZ	No. of probe locations (up to 8)
ZOUT(1-NHTZ)	Probe AXIAL LOCATION(s) for output (in)

Card 7: Radial Probe Location

ROUT(1-NHTZ)	Probe RADIAL LOCATION(s) from inside surface (in)

Card 8: Erosion Material (Base) and Numerical Information

ICHEM	1 equilibrium, 0 none, 2 finite rate kinetics on surface and equilibrium subsurface (-)
TFREEZ	Surface routine freeze out temperature (K)
RHOSTEEL	Density of the wall material (kg/m^3)
TMELT	Temperature at which the material begins to melt (K)
CHTOUT	Outer barrel heat transfer coefficient ($W/m^2/K$)
TOUT	Ambient outer air temperature (K)
DETA	Computational coordinate spacing (-) usually "1"
HOF	Latent heat of fusion for the material (J/kg)
IAXI	"0" if the system is planer or "1" if the system is axisymetric
MTMIX	Surface temperature (1) Molecular weighting function (2) Wall temperature

Conditional Card 2: Erosion Material (Coating) and Numerical Information (if chrome > 0)

NCOAT	Number of radial points in coating material (-)
NBASE	Number of radial points in base material (-)
TFREEZC	Coating freeze-out temperature (K)
RHOCOAT	Coating density (Kg/m^3)
TMELTC	Melting temperature of coating (K)
DETA	Computational coordinate spacing (-) usually "1" (-)
HOFC	Latent heat of fusion for coating material (J/kg)
SCALC	Coating Stress Flag (-)

Conditional Card 3: Stress Calculation Card (if SCALC >= 1)

YMC	Young's Modulus Coating (Pa)
CTEC	Coefficient of Thermal Expansion Coating (1/K)
PRC	Poisson's Ratio Coating (-)
USC	Ultimate Strength of Coating (Pa)
YMB	Young's Modulus Base (Pa)
CTEB	Coefficient of Thermal Expansion Base (1/K)
PRB	Poisson's Ratio Base (-)

Conditional Card 4: Surface Crack Card (if SCALC > 1)

CW	Crack Width (m)
CLIMIT	Crack Distribution Limit for Heat Transfer Augmentation (m)

Card 9: Burst Fire, Numerical Time Step, and Print Control

NROUNDS	No. of rounds to be simulated

(NOT IMPLEMENTED IN THIS VERSION = 1)

NKOUNT1	Counter for output print intervals (during htemp.out for each round)
NKOUNT2	Counter for output print intervals (after htemp.out for each round)
DELTV	Numerical time step (s)
LASTSHOT	Last round of the immediately previous simulation

(NOT IMPLEMENTED IN THIS VERSION = 0)

Card 10: Output File Control (0 = false), (1 = true), (2 = >single shot = burst)

IUNIT	Units to be printed 0=K, 1=R	
ITEMP	Temperature 0 = as computed, 1= temperature rise	
IOUT(1)	Screen output	
IOUT(2)	Single shot probe temperature	(NHTZ locations)
IOUT(3)	Single shot inside surface temperature	(NHTZ locations)
IOUT(4)	Single shot outside surface temperature	(NHTZ locations)
IOUT(5)	Burst fire probe temperature	(NHTZ locations)
IOUT(6)	Burst fire inside surface temperature	(NHTZ locations)
IOUT(7)	Burst fire outside surface temperature	(NHTZ locations)

IOUT(8)	Heat transfer coefficient	(NHTZ locations)
IOUT(9)	Effective gas temperature history	(NHTZ locations)
IOUT(10)	Single shot graphic output file	(for IBGRAF)
IOUT(11)	Burst fire graphic output file	(for IBGRAF)
IOUT(12)	Boundary condition output file (P,T,U, I.B.)	(for IBGRAF)
IOUT(13)	Bore surface heat flux output file	(NHTZ locations)
IOUT(14)	Bore surface regression rate	(NHTZ locations)
IOUT(15)	Bore surface regression	(NHTZ locations)
IOUT(16)	Bore surface concentrations	(NHTZ locations)
IOUT(17)	Bore core flow concentrations	(NHTZ locations)
IOUT(18)	Shear stress azmuthal at interface	(NHTZ locations)
IOUT(19)	Shear stress axial at interface	(NHTZ locations)

(Note: Screen output is for PC applications only and is not supported.)

Card 11: Barrel Material Properties

IF4340	(1 = true; 0 = false)
XKS	Conductivity of barrel (W/m/K)
	(if IF4340 = 1, a number must still be entered here)
ALFAS	Diffusivity of barrel (m^2/s))
	(if IF4340 = 1, a number must still be entered here)
XKC	Conductivity of liner (W/m/K)
ALFAC	Diffusivity of liner (m^2/s)

Card 12: Chemistry Data Flag (-)

AMAGIC "42" – key flag number for the chemistry reading section (-)

Card 13: Chemistry Data Flag (A30)

TITLE: Key phrase for chemistry read section

"NUMBER OF REACTANT ELEMENTS = "

Card 14: Chemistry Data Card (I3)

NEL: Number of reactant elements (-)

Card 15: Chemistry Data Flag (A30)

TITLE: Key phrase for chemistry read section

"CONSIDERED ELEMENTS = "

Card 16: Chemistry Data Card (10A4)

CELEM2(NN) – Element symbols

Card 17: Chemistry Data Flag (A30)

TITLE: Key phrase for chemistry read section

"REACTANTS"

Card 18 + No. of Reactants: Chemistry Data Cards (5A4,4(A2,F3.0),A1)

19.1–19.7

CNAME(N,K):	Enter the reactant species name (left justified) as it appears in the N-L library.
OSPEC1(N,J)	Elemental symbol (left justified)
OSPEC2(N,J)	Number of elements in reactant
ORFAZ(N)	Phase: "G", "L", or "S"
PCRIT(N)	Critical Pressure (Pa)
TCRIT(N)	Critical Temperature (K)
SIGMA(N)	Sigma for Lennard Jones diffusion (Å)
EPSOK(N)	Epsilon over K EPSOK for Lennard Jones diffusion (K)

Continue until all reactants have been entered # = MXGAS

Card 19: Chemistry Data Flag (A30)

TITLE: Key for chemistry read section

"PRODUCTS"

Card 20 + No. Products: Chemistry Data Cards (5A4,4(A2,F3.0),A1)

20.1–20.7

CNAME(N,K):	Enter the reactant species name (left justified) as it appears in the N-L library.
OSPEC1(N,J)	Elemental symbol (left justified)
OSPEC2(N,J)	Number of elements in reactant
ORFAZ(N)	Phase: "G", "L", or "S"
PCRIT(N)	Critical Pressure (Pa)

TCRIT(N)	Critical Temperature (K)
SIGMA(N)	Sigma for Lennard Jones diffusion (Å)
EPSOK(N)	Epsilon over K EPSOK for Lennard Jones diffusion (K)

Continue until all products have been entered # = MXGAS

Kinetics data input follows:

Conditional Card 5: Kinetics Title Card (A40) (if ICHEM = 2)

TITLEK	Key phrase for kinetics read section
	"KINETICS BEGIN REACTION CARDS'

Conditional Card 6: Kinetics Data Card (3I5) (if ICHEM = 2)

KNSPEC	Number of species
NRXN	Number of reactions

Conditional Card 7: Kinetics Data Card (4(5A4) (if ICHEM = 2)

CSPECK(NN,J)	Character array of considered species names (Order is important)

Conditional Card 8: Reactants Title & Data Card (A40) (if ICHEM = 2)

TITLEK	Key phrase for kinetics read section
	"CONSIDERED SPECIES FOR KINETIC REACTIONS"

Conditional Card 9: Reactants Name Card (4(5A4)) (if ICHEM = 2)

CSPECK	Species characters using NASA Lewis notation, using as many lines as needed

Conditional Card 10: Data Card (A10,6E10.4,F5.0,I5) (if ICHEM = 2)

TITLESMALL	Key phrase for kinetics read section
	"REACTANTS"
CF(N)	Forward rate coefficient (cm^3/mole-s) or (cm^6/mole^2-s)
ETAF(N)	Forward rate temperature exponent ETAF (-)
EF(N)	Forward rate activation energy EF/k (K)
CB(N)	Backward rate coefficient (cm^3/mole-s) or (cm^6/mole^2-s)
	"0" - not considered, "-1" computed from thermodynamics
ETAB(N)	Backward rate temperature exponent ETAB (-)
	"0" - not considered, "-1" computed from thermodynamics

EB(N), Backward rate activation energy EB/k(K)

"0" - not considered, "-1" computed from thermodynamics

BODY3(N) Third body flag (1=T, 0=F)

ICOFU(N) Surface or gas phase reaction flag (0 NORMAL 1 = SURFACE)

Kinetic reactant and product data cards for reaction follow:

Conditional Card 11: Reactants Data Card (5A4,F3.0,4(A2,F3.0),A1,4E10.4) (if ICHEM = 2)

CKNAME(N,M,K),K=1,5) First reactant of reaction using NASA Lewis Notation

CRCTT(N,M) Reactant atomic coefficient

OSPECK1(N,M,J) Reactant atomic character

OSPECK2(N,M,J),J=1,4) Corresponding reactant atomic subscript

ORFAZK(N,M) Reactant phase "G", "S", "L"

Continue with Card 11 until all reactants in reaction are entered.

Conditional Card 12: Products Flag Card (5A4,F3.0,4(A2,F3.0),A1)

(if ICHEM = 2)

CKNAME(N,M,K),K=1,5) Key phrase for kinetics read section

"PRODUCTS"

Conditional Card 13: Products Data Card (5A4,F3.0,4(A2,F3.0),A1,4E10.4)

(if ICHEM = 2)

CKNAME(N,M,K),K=1,5) First product of reaction using NASA Lewis Notation

CRCTT(N,M) Product Atomic Coefficient

OSPECK1(N,M,J) Product atomic character

OSPECK2(N,M,J),J=1,4) Corresponding reactant atomic subscript

ORFAZK(N,M) Product phase "G", "S", "L"

Continue with Card 13 until all products in reaction are entered.

Conditional Card 14: Efficiency Flag Card (5A4,F3.0,4(A2,F3.0),A1)

(if BODY3 = 1)

CKNAME(N,M,K),K=1,5) Key phrase for kinetics read section

"EFFICIENCY"

Conditional Card 15: Efficiency Data Card (7E10.4) (if BODY3=1)

EFF(N,J) Efficiency of each species CSPECK (in CSPECK order!) reacting with each other species (in CSPECK order!) to make a product.

Conditional Card 16: End of Kinetic Reaction Card (5A4,F3.0,4(A2,F3.0),A1)

(if BODY3 not equal to 1)

KEND Key phrase for kinetics read section after each reaction if it is not a third body

"KEND"

Continue looping on conditional Cards 10–16 until all reactions are entered.

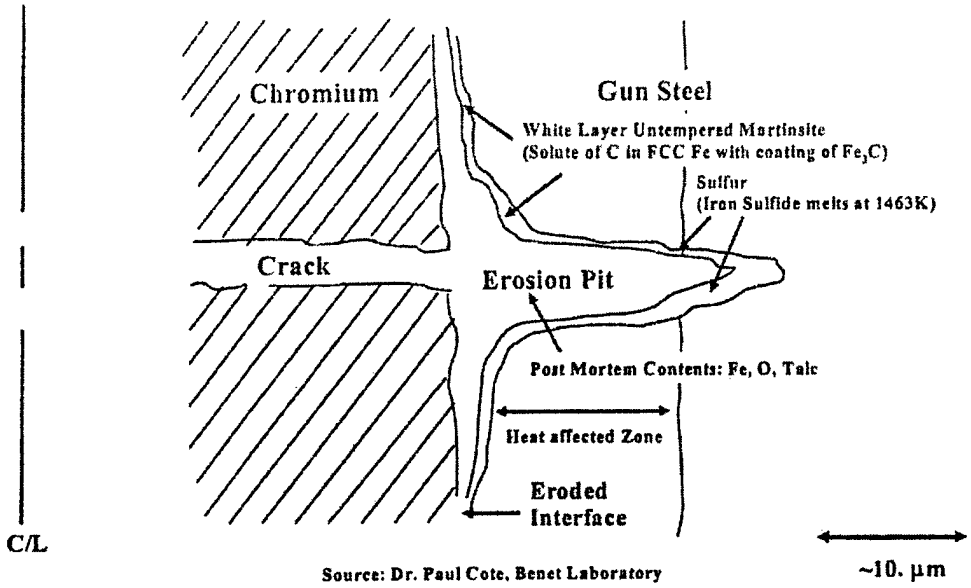

Figure 1. Description of post-mortem erosion pit.

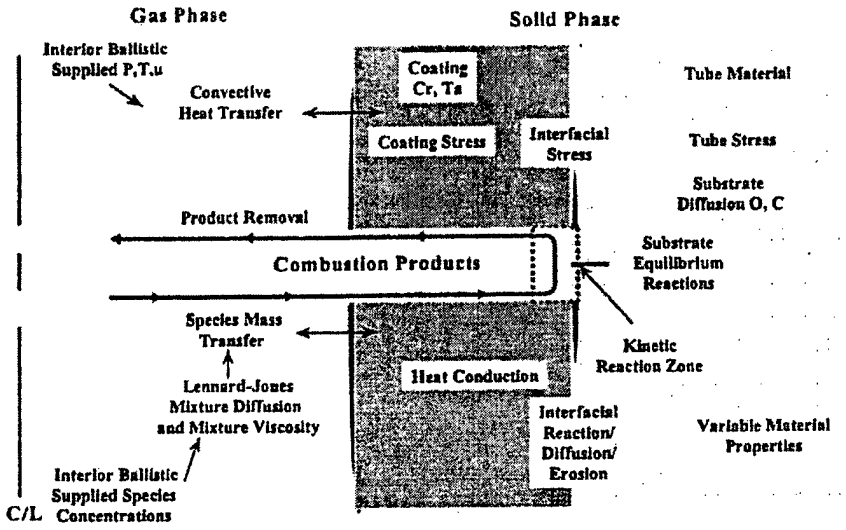

Figure 2. Analytical surface coating description including stress.

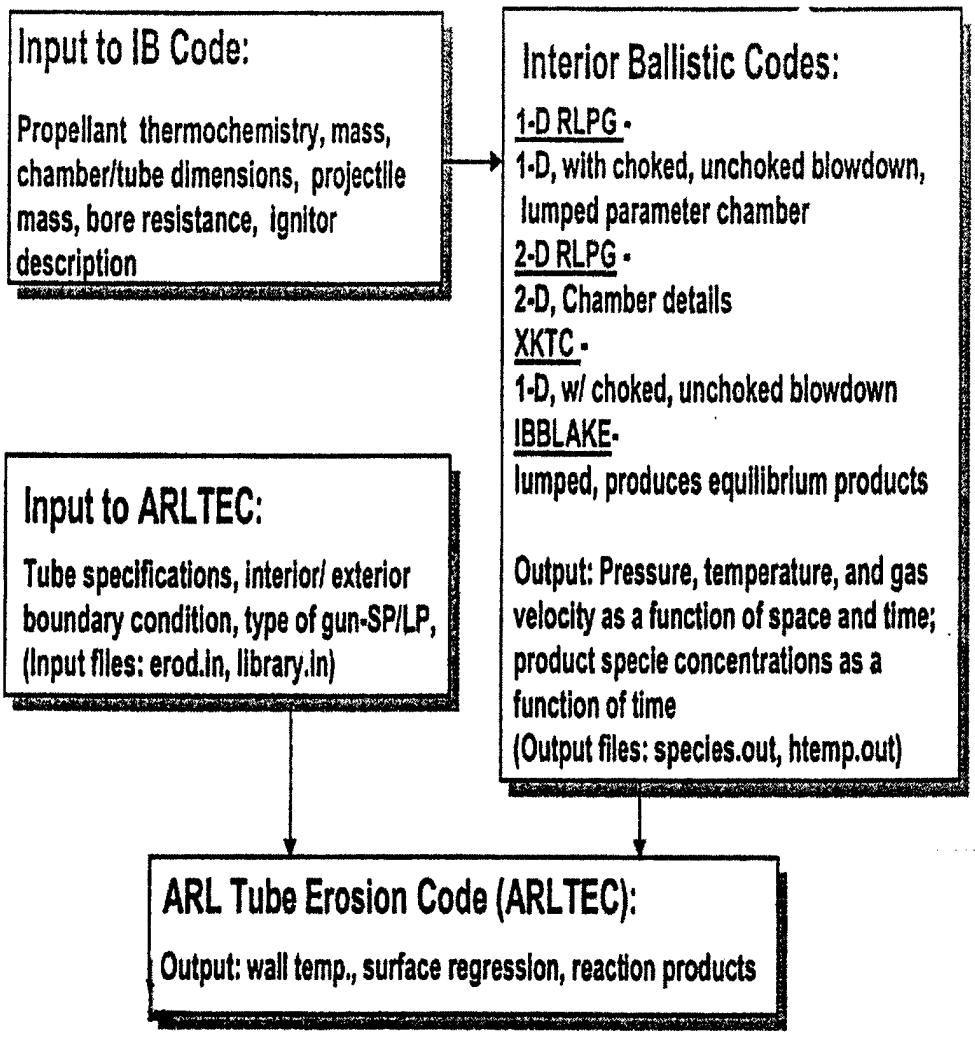

Figure 3. Code/file connectivity.

Table 1. ATEC input/output file table.

"EK58.f" file numbering table				
File No.	File name	Purpose	Input	Output
8	htcoff.dat	Heat transfer coefficient data		X
9	bprobe.dat	Residual probe data (burst)		X
10	ssurfi.dat	Single (burst) shot bore temperature		X
11	bsurfo.dat	Residual (burst) outer surface temperature		X
12	LASTTEMP.DAT	Restart data file	X	X
15	erod.in	User input	X	
16	erod.out	Echo of user input		X
17	scratch	–		X
20	sprobe.dat	Single (burst) shot probe temperature		X
21	ssurfi.dat	Single (burst) shot bore temperature		X
22	ssurfo.dat	Single (burst) outer surface temperature		X
23	htemp.out	IB input	X	
24	LASTTEMP.DAT	Restart data file	X	X
25	gastmp.dat	Effective gas temperature for exported B.C.		X
27	stemps.tab	Single (burst) graphic probe temperatures		X
28	btemps.tab	Burst, graphic probe temperatures		X
29	sputib.tab	Single (burst) graphic P,T,u output (tableaux)		X
30	species.out	Species file from IBBLAKE	X	
32	library.in	NASA Lewis Library	X	
33	–	–	–	–
34	intp.out	Interpolated species concentration output		X
35	senergy.dat	Bore heat flux convection/chemical		X

Table 1. ATEC input/output file table (continued).

"EK58.f" file numbering table				
File No.	File name	Purpose	Input	Output
36	sdsdt.dat	Bore surface regression rate		X
37	sregres.dat	Bore surface regression		X
38	surfphi.dat	Bore surface concentrations		X
39	corephi.dat	Bore core flow concentrations		X
40	shears.dat	Shear stress azmuthal at interface		X
41	shearz.dat	Shear stress axial at interface		X
	fort.3	Input echo		X
	test.out	Diagnostics information		X

6. References

1. Conroy, P. J., P. Weinacht, and M. J. Nusca. "Surface Chemistry Effects on High Performance Tank Ammunition." ARL-TR-1526, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, October 1997.
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3. Conroy, P. J., P. Weinacht, and M. J. Nusca. "Erosion: A Parametric Study—Flame Temperature." Submitted to the *Journal of Defense Science*, April 2000.
4. Conroy, P. J., P. Weinacht, and M. J. Nusca. "Gun Tube Coatings in Distress." ARL-TR-2393, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, February 2001.
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7. Weinacht, P., and P. J. Conroy. "A Numerical Method for Predicting Thermal Erosion in Gun Tubes." ARL-TR-1156, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, October 1996.
8. Gough, P. S. "The XNOVAKTC Code." BRL-CR-627, U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, 1990.
9. Gordon, S., and B. J. McBride. "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouget Detonations." NASA SP-273, NASA Lewis, Cleveland, OH, 1971.
10. Cote, P. J., and C. Rickard. "Gray Layers and the Erosion of Chromium Plated Gun Bore Surfaces." Submitted to *WEAR*, August 1999.
11. Fisher, R. M., A. Sizrmae, and M. H. Kamdar. "Metallographic Studies of Erosion and Cracking of Cannon Tubes." *Proceedings of the Tri-Service Gun Tube Wear and Erosion Symposium*, pp. II-151–II-160, U.S. Army Armament Research, Development, and Engineering Center, Picatinny Arsenal, Dover, NJ, October 1982.

Appendix A. Example Input Number 1

This appendix appears in its original form, without editorial change.

```
;;-------------------------------------------------------------------------
;; Example Input Number 1, June 2001
;;-------------------------------------------------------------------------
;  NOTES:
;
;    - Add as many comment lines as you want.
;    - Each comment line *must* have a semi-colon in column 1.
;    - Add comment lines carefully. Most common error is to put a colon (:)
;      instead of a semi-colon (;) in column 1. Erosion program issues warning
;      message and continues.
;    - Can include blank lines
;    - Those comments that have a semi-colon in column 2 as well are echoed in the
;      output file ero.out (like the first three lines of this file.
;    - The free format is nice to use but some systems do not permit more than 72
;      characters per line.
;;
; Please use "instructions" pamphlet to ensure correct input deck development
;-------------------------------------------------------------------------
; Ambient Temp (R), Pr (psi), gas vel (in/s)    (FROM XKTC FILE: htemp.out)
;  :    ..............:            :          (CRUMMY UNITS ARE FROM THE 70'S)
;  :    :    ......................:
;  :    :    :

530.0 14.70 0.00
```

```
;-------------------------------------------------------------------------
; xchrom (in), tmaxv (ms), xcon, xcham (in),
;  :      .........:         :      :
;  :      :      ..............:      :
;  :      :      :     ................:
;  :      :      :     :
;  :      :      :     :    zmax (in) , nloc , zstart (in), zend (in)
;  :      :      :     :     :      ......:         :          :
;  :      :      :     :     :      :     ............:          :
;  :      :      :     :     :      :     :     ..................:
;  :      :      :     :     :      :     :     :  2-D LP chamber option
;  :      :      :     :     :      :     :     :     :   piston offset for 2-D LP calculation (initial)
;  :      :      :     :     :      :     :     :     :     :   IMC (extra card required at end)
;  :      :      :     :     :      :     :     :     :     :     :   insulate outer B.C.
;  :      :      :     :     :      :     :     :     :     :     :     :   blowby (extra card need placed at end)
;  :      :      :     :     :      :     :     :     :     :     :     :     :           (after IMC card if present)
;  :      :      :     :     :      :     :     :     :     :     :     :     :   heat XFR coefficient fudge factor
;  :      :      :     :     :      :     :     :     :     :     :     :     :     :
;  :      :      :     :     :      :     :     :     :     :     :     :     :     :<72

0.000   15.0  0.0  7.0  14.0   16  7.6 10.6   NA   NA   NA   NA   NA 1.  Standard heat transfer
;0.010  15.0  0.0  22.0  200.   3  25.  28.   NA   NA   NA   NA   NA -1.  Augmented heat transfer

;  ROUGHNESS DATA  (only if heat transfer coefficient fudge factor is negative)
;  esmooth (m) smooth deformation limit (Moody chart)
;  :           erough (m) rough deformation limit (Moody chart)
;  :           :

;   1.524D-6   5.D-2

; ESMOOTH = 2.540D-4      ! (m) CHROME THICKNESS - CHIPPED VIRGIN TUBE
; ESMOOTH = 1.5240D-6     ! (m) DRAWN TUBING - CHROMED TUBE VIRGIN
; EROUGH  = 5.0D-2        ! (m) CONDEMNATION CRITERA FOR M256 = 0.5cm therefore EROUGH larger than limit

; Barrel Geometry :
; ndtz, zdb (1:ndtz) -- no of axial locations, ndtz locations (in)
; (max = 8)
;     1      2      3      4      5      6      7      8

8   0.0  5.870  6.500  8.877  8.927  9.027  9.370   10.5
```

```
; dbar (1:ndtz)       -- barrel o.d. at ndtz locations (in)

   4.00   4.00   4.00   4.00   4.00   4.00   4.00   4.00

; dbor (1:ndtz)       -- barrel i.d. at ndtz locations (in)
;     1      2      3      4      5      6      7      8

   1.972  1.942  1.532   0.73  0.618  0.538   0.49   0.50

; Desired Output Locations:
;-------------------------------------------------------------------------
; nhtz, zout (1:nhtz)-- no of locations for output, nhtz locations (in)
; (max =8)
;
;   1      2      3      4      5      6      7      8

8 8.90   9.00   9.10   9.20   9.30   9.37   9.50   9.60

; rout (1:nhtz)       -- radial depth at nhtz locations (in)
;   1      2      3      4      5      6      7      8

 0.010  0.010  0.010  0.010  0.010  0.010  0.010  0.010

;
; EROSION DATA CARD (BASE MATERIAL!)
;  .... ICHEM  (2) EQUILIBRIUM AND KINETICS ON (1) EQUILIBRIUM ONLY ON (0) OFF
;  :    .... FREEZE-OUT TEMPERATURE (i.e. ICHEM=0) (K)
;  :    :       .....  DENSITY IN (kg/m3)
;  :    :       :       ......MELT TEMP (K)
;  :    :       :       :      .......OUTER BARREL HEAT TRANSFER COEF (W/m2/K)
;  :    :       :       :      :     ..... AMBIENT AIR TEMP (K) (OUTSIDE)
;  :    :       :       :      :     :     ..... COMPUTATIONAL COORD SPACING (-)
;  :    :       :       :      :     :     :     ..... LATENT HEAT OF FUSION (J/kg)
;  :    :       :       :      :     :     :     :      .... (0) PLANER (1) AXISYMETRIC
;  :    :       :       :      :     :     :     :      :  .... TMIX control volume temperature flag
;  :    :       :       :      :     :     :     :      :  :          (1)Molecular weighting function
;  :    :       :       :      :     :     :     :      :  :          (0)Wall temp
;  :    :       :       :      :     :     :     :      :  :
;  :    :       :       :      :     :     :     :      :  :

   2  550.0  7827.0  2720.0  6.0  298.0  1.0  2.7E+5  1  0
```

```
; EROSION COATING DATA CARD ONLY IF CHROME > 0.D0
;   ...NUMBER OF RADIAL PTS IN COATING (-)
;   :     .....NUMBER OF RADIAL PTS IN BASE MATERIAL (-)
;   :     :     .... FREEZE-OUT TEMPERATURE (i.e. ICHEM=0) (K)
;   :     :     :      ..... DENSITY IN (kg/m3)
;   :     :     :      :      ......MELT TEMP (K)
;   :     :     :      :      :      ..... COMPUTATIONAL COORD SPACING (-)
;   :     :     :      :      :      :     .... LATENT HEAT OF FUSION (J/kg)
;   :     :     :      :      :      :     :      ...COATING STRESS FLAG (-)
;   :     :     :      :      :      :     :      :
;   :     :     :      :      :      :     :      :
;   :     :     :      :      :      :     :      :
;   :     :     :      :      :      :     :      :

;   35    65    250.0  16650.0 3269.  1.0  1.7E+5   1      Ta
;   35    65    250.0  7827.0  2133.0  1.0  2.7E+5  1     chrome

;  COATING STRESS CALCULATION CARD - ONLY IF COATING STRESS FLAG GT 0
;       .... Youngs Modulus Coating (Pa)
;       :     .... CTE Coating (1/K)
;       :     :     .... Poisson's Ratio Coating (-)
;       :     :     :     .... Ultimate Strength Coating (Pa)
;       :     :     :     :     .... Youngs Modulus Base (Pa)
;       :     :     :     :     :     .... CTE Base(1/K)
;       :     :     :     :     :     :     .... Poisson's Ratio Base (-)
;       :     :     :     :     :     :     :
;
;    186.D9  6.8D-6  0.35D0  900.D6  211.D9 12.6D-6  .296D0
;     TA      TA      TA      TA     4340    4340    4340
;   248.D9  6.5D-6  0.21D0  413.D6  211.D9 12.6D-6  .296D0
;  chrome  chrome  chrome   chrome   4340    4340    4340

;  chrome data from www.matweb.com
;  4340 data from 4340 material data sheet

;  CRACK CALCULATION CARD - ONLY IF COATING STRESS FLAG GT 0
;     ....  Crack Width (m)
;     :     ....  Crack Distribution Limit (m) for augmentation of HXF in crack
;     :     :
;  2.D-4     50.0
;
```

```
;  crack width - estimated
;  crack distribution limit - estimated

; Firing Data:
;-------------------------------------------------------------------------------
; nrounds, nkount1, nkount2, deltv (s), lastshot
;   ..........:       :            :       :
;   :    ............:            :       :
;   :    :      .....................:       :
;   :    :      :    ......................:
;   :    :      :    :

1   5   20   10D-6   0
```

```
; Desired Output Units and Files:
;-------------------------------------------------------------------------------
;
; iunit (0 for K, 1 for deg R) Units flag
;   ___ itemp (0 for as calculated, 1 for temp rise),
; |
; |  _______. screen output                                  (single shot-1, burst-2)          IOUT(1)
; | |                                        iout (1:9) ---
; | | _______ single shot probe temperature,                                                    IOUT(2)
; | | |_______single shot inside surface temperature,                                          IOUT(3)
; | | | ______single shot outside surface temperature,                                        IOUT(4)
; | | | |
; | | | | _____ burst fire probe temperature,                                                  IOUT(5)
; | | | | |____ burst fire inside surface temperature,                                       IOUT(6)
; | | | | | |___ burst fire outside surface temperature,                                     IOUT(7)
; | | | | | | |
; | | | | | | | ___ heat transfer coefficient,                                               IOUT(8)
; | | | | | | | |___ effective gas temperature history                                       IOUT(9)
; | | | | | | | | |
; | | | | | | | | | ___ single shot graphics output (for IBGRAF movies)                      IOUT(10)
; | | | | | | | | | |___  burst fire graphics output (for IBGRAF movies)                       IOUT(11)
; | | | | | | | | | | |___ boundary condition graphic output (for IBGRAF movies)               IOUT(12)
; | | | | | | | | | | |
; | | | | | | | | | | | ___ bore surface heat flux output                                        IOUT(13)
; | | | | | | | | | | | |___ bore surface regression rate                                        IOUT(14)
; | | | | | | | | | | | | |___ bore surface regression                                           IOUT(15)
; | | | | | | | | | | | | | |__ core species concentration (-)                                     IOUT(16)
; | | | | | | | | | | | | | | |__ wall species concentrations(-)                                   IOUT(17)
; | | | | | | | | | | | | | | | |__ interfacial shear (MPa)                                          IOUT(18)
; | | | | | | | | | | | | | | | | |__ interfacial axial shear (MPa)                                  IOUT(19)
; | | | | | | | | | | | | | | | | | |__ blank                                                        IOUT(20)
; | | | | | | | | | | | | | | | | | | |

0 0 0 0 2 0 0 0 0 2 2 0 0 0 0 0 2 0 0 0 0 0
;   1 2 3 4 5 6 7 8 9101112131415161718192 0

  Variable   Property: k Barrel    Alpha Barrel      k Liner    Alpha Liner
;  Property   Material:   (4340)          (4340)       (4340)          (4340)
;  For 4340   Units:     (W/m/K)          (m2/s)       (W/m/K)         (m2/s)
; (1=y,2=no)  Source:     [TPOM]          [TPOM]         [I&D]          [I&D]
       1                   34.1         5.7e-6         34.1         5.7e-6
```

```
; Note: The variable property option overrides the other property inputs Alpa,Cp
; New physical property inputs are in units of W,m,s,K (only for version v32 and above)

;  Material       Data Source                Value          @Temp      MKS Units
; 304SS k  pg. 1164 curve 11 TPOM Vol. 1    0.180  W/cm/K @523K  = 18.0 W/m/K
; 304SS k  pg. 1164 curve 11 TPOM Vol. 1    0.219  W/cm/K @823K  = 21.9 W/m/K
; 4340  k  pg. 1212 curve 21 TPOM Vol. 1    0.335  W/cm/K @295K  = 33.5 W/m/K
; 4340  k  pg. 1212 curve 25 TPOM Vol. 1    0.341  W/cm/K @813K  = 34.1 W/m/K
; CHROME k pg. 755  Inc. and Dewitt         0.807  W/cm/K @ 600K = 80.7 W/m/K
; CHROME k pg. 755  Inc. and Dewitt         0.654  W/cm/K @1000K = 65.4 W/m/K
; Comp. k11 = k22 Tzeng Comp. Man. V4 #3    0.0071 W/cm/K        = 0.71 W/m/K
; Comp. k33 Tzeng       Comp. Man. V4 #3    0.160  W/cm/K        = 16.0 W/m/K
; 304SS   g. 344  curve 11 TPOM Vol.10    0.0352 cm2/s @ 460K  = 3.52e-6 m2/s
; 304SS   g. 344  curve 11 TPOM Vol.10    0.0457 cm2/s @1146K  = 4.57e-6 m2/s
; 4340    g. 362  curve 2  TPOM Vol.10    0.096  cm2/s @ 313K  = 9.6e-6  m2/s
; 4340    g. 362  curve 3  TPOM Vol.10    0.087  cm2/s @ 313K  = 8.7e-6  m2/s
; 4340    g. 362  curve 3  TPRC Vol.10    0.057  cm2/s @1203K  = 5.7e-6  m2/s
; CHROME  . 755  Inc. and Dewitt          0.207  cm2/s @ 600K  = 2.0795e-5m2/s
; CHROME  . 755  Inc. and Dewitt          0.148  cm2/s @1000K  = 1.4828e-5m2/s
; Composite Tzeng Comp. Manu. Vol 4 no 3    0.0051 cm2/s          = 5.10e-7 m2/s
; Composite Tzeng Comp. Manu. Vol 4 no 3    0.1150 cm2/s          = 1.15e-5 m2/s
```



```
42
This species input section is keyed on key phrases in the following notes:
Also the previous number "42" is a "magic number" flag
1.SPECIES NAME MUST MATCH NASA LEWIS LIBRARY NAME EXACTLY
2.LEFT JUSTIFIED ELEMENT CHARACTERS
3.RIGHT JUSTIFIED ELEMENT NUMBERS
4.FORMAT (5A4,4(A2,F3.0),A1)
5.LEAVE EXTRAINIOUS FORMAT SEGMENTS BLANK
6.PHASE MUST BE EXPLICITLY SPECIFIED
7.REACTANT ORDER MUST BE THE SAME AS THAT EXTRACTED FROM IB CODE
8.KEY POINTER PHRASES ARE:
FORMAT(A30,I3):                    "NUMBER OF REACTANT ELEMENTS = ",#
CONSIDERED ELEMENTS IN "A" ORDER: "CONSIDERED ELEMENTS = "
BEGINING OF ALL REACTANT CARDS:    "REACTANTS"
BEGINING OF THE PRODUCT CARDS:     "PRODUCTS"

NUMBER OF REACTANT ELEMENTS =
8
```

```
CONSIDERED ELEMENTS =
H   C   N   O   S   CR  FE  NI
REACTANTS
;       FORMAT (5A4,4(A2,F3.0),A1,4E10.4)
;FORMULA            ELEMENTS,#      PHASE PCRIT(Pa)  TCRIT(K)  SIGMA(A) EPSOK(K)
;A4][A4][A4][A4][A4][][ ][][ ][][ ][][ ]A[ E10.4  ][  E10.4 ][ E10.4  ][ E10.4 ]
H2                  H   2               G     1.3E6      33.1     2.827   59.7
O2                  O   2               G    5.08E6     154.6     3.467  106.7
CO                  C   1O   1          G     3.5E6      133.0     3.690   91.7
CO2                 C   1O   2          G    7.39E6      304.0     3.941  195.2
H2O                 H   2O   1          G   22.09E6      647.1     2.641  809.1
SO2                 S   1O   2          G    7.88E6      430.8     4.112  335.4
N2                  N   2               G    3.39E6      126.0     3.798   71.4
NO                  N   1O   1          G    6.48E6      180.0     3.492  116.7
; note: the 1RST solid reactant (9th reactant) must be C(GR) solid phase
C(GR)               C   1               S       1.0        1.0       1.0     1.0
; note: the 10th reactant must be FE(A) solid phase
FE(A)               FE  1               S       1.0        1.0       1.0     1.0 10
; note: the 11th reactant must be FE(C) solid phase
FE(C)               FE  1               S       1.0        1.0       1.0     1.0 11
NI(B)               NI  1               S       1.0        1.0       1.0     1.0 12
S                   S   1               G       1.0        1.0       1.0     1.0 13
CR2O3(S)            CR  2O   3          S       1.0        1.0       1.0     1.0 14
PRODUCTS
; note: FE3C must be the 15th (reactant+product) to match index in program
FE3C                FE  3C   1          S       1.0        1.0       1.0     1.0    15
FEO(S)              FE  1O   1          S       1.0        1.0       1.0     1.0    16
FE3O4(S)            FE  3O   4          S       1.0        1.0       1.0     1.0    17
FE2O3(S)            FE  2O   3          S       1.0        1.0       1.0     1.0    18
FEO(L)              FE  1O   1          L       1.0        1.0       1.0     1.0    19
FE                  FE  1               G       1.0        1.0       1.0     1.0    20
FE(L)               FE  1               L       1.0        1.0       1.0     1.0    21
FEO                 FE  1O   1          G       1.0        1.0       1.0     1.0    22
FEO2H2              FE  1O   2H   2     G       1.0        1.0       1.0     1.0    23
H                   H   1               G       1.0        1.0       1.0     1.0    24
O                   O   1               G       1.0        1.0       1.0     1.0    25
; Note:  Neither the critical values nor the Leonard Jones values for O and H in
;       substrate.  This influences neither the surface state nor transport calculation
NO2                 N   1O   2          G       1.0        1.0       1.0     1.0    26
NI(L)               NI  1               L       1.0        1.0       1.0     1.0    27
OH                  O   1H   1          G       1.0        1.0       1.0     1.0    28
```

```
;S2                  S   2                    G       1.0       1.0       1.0       1.0     25 -
;COS                 C   1O   1S   1          G       1.0       1.0       1.0       1.0     26 -
;SO                  S   1O   1               G       1.0       1.0       1.0       1.0     27 -
;CRO                 CR  1O   1               G       1.0       1.0       1.0       1.0     28 -
;CRO2                CR  1O   2               G       1.0       1.0       1.0       1.0     29 -
;HCO RAD             H   1C   1O   1          G       1.0       1.0       1.0       1.0     30 -
;HCN                 H   1C   1N   1          G       1.0       1.0       1.0       1.0     31 -
;HNO                 H   1N   1O   1          G       1.0       1.0       1.0       1.0     32 -
;OH+                 O   1H   1E -1.          G       1.0       1.0       1.0       1.0     15 -
;NIO2H2              NI  1O   2H   2          G       1.0       1.0       1.0       1.0     35 -
;NI                  NI  1                   G       1.0       1.0       1.0       1.0     36 -
;NIO                 NI  1O   1               G       1.0       1.0       1.0       1.0     37 -
EQEND
;    SIGMA, EPSOK,    SOURCE    - MARTIN MILLER'S BOOK AND HIRSHFIELDER
;    TCRIT, PCRIT,    SOURCE    - VAN WEHLAN AND SONNTAG

;------- Kinetics data follows-----------------------------------------------------------------
KINETICS BEGIN REACTION CARDS
;   ..NUMBER OF KINETIC REACTANT SPECIES (-) FORMAT(4(5A4))
;   :    ..NUMBER OF REACTIONS            (-)
;   :    :
   10    7

CO2                  CO                   O2                   C(GR)
FE(A)                O                    H2O                  H2
H                    OH

CONSIDERED SPECIES FOR KINETIC REACTIONS
;         .. REACTANTS "KEY WORD" FORMAT(A10,7E10.4,I5)
;         :          ..  CF (cm^3/mole-s) or (cm^6/mole^2-s) FORWARD RATES
;         :          :          ..ETAF (-)
;         :          :          :          .. EF/k (K) (0 => NOT CONSIDERED, -1 => COMPUTED)
;         :          :          :          :     (cal -> need ICOFU=1)
;         :          :          :          :          .. CB (cm^3/mole-s) or (cm^6/mole^2-s) REV RATES
;         :          :          :          :          :          .. ETAB (-)
;         :          :          :          :          :          :          .. EB/k(K) (0=>NOT,-1=>THERMO)
;         :          :          :          :          :          :          :     .. THIRDBODY (-)
;         :          :          :          :          :          :          :     :    (1=T, 0=F)
;         :          :          :          :          :          :          :     :    ..ICOFU (-)
;         :          :          :          :          :          :          :     :    :  (0 NORMAL 1 = SURFACE)
;         :          :          :          :          :          :          :     :    :
```

```
;1RST REACTION    CO + O <-> CO2    3rd order rxn
REACTANTS    6.17E14       0.0    1510.0       0.0       0.0       0.0  1.0    0
;   FORMAT (5A4,F3.0,4(A2,F3.0),A1,4E10.4)
CO                     1C   1O   1          G
O                      1O   1               G
PRODUCTS
CO2                    1C   1O   2          G
EFFICIENCY
;  FORMAT (7(F10.0))
       1.0       1.0       1.0       1.0       1.0       1.0       1.0
       1.0       1.0       1.0

;2ND REACTION  CO + Fe <-> Fe + C + O
REACTANTS     5.2E14       0.0   23903.0       0.0       0.0       0.0  0.0    0   works for 120mm gun
CO                     1C   1O   1          G
FE(A)                  1FE  1               S
PRODUCTS
O                      1O   1               G
C(GR)                  1C   1               S
FE(A)                  1FE  1               S
;note: if NOT 3rd body RXN, "KEND" is required at end of reaction
KEND

;3RD REACTION     O + O <-> O2
REACTANTS    1.89E13       0.0    -900.0       0.0       0.0       0.0  1.0    0
O                      2O   1               G
PRODUCTS
O2                     1O   2               G
EFFICIENCY
       1.0       1.0       1.0       1.0       1.0       1.0       1.0
       1.0       1.0       1.0

;4RTH REACTION  H + OH <-> H2O
REACTANTS    8.35E21      -2.0       0.0       0.0       0.0       0.0  1.0    0
OH                     1O   1H   1          G
H                      1H   1               G
PRODUCTS
H2O                    1H   2O   1          G
EFFICIENCY
       1.0       1.0       1.0       1.0       1.0       1.0       1.0
       1.0       1.0       1.0
```

```
;5TH REACTION  H2 + FE <-> H + H + FE
REACTANTS     4.57E19       -1.4    52530.0        0.0        0.0        0.0  0.0     0
H2                      1H   2                 G
FE(A)                   1FE  1                 S
PRODUCTS
FE(A)                   1FE  1                 S
H                       2H   1                 G
KEND

;6TH REACTION  H + O <-> OH
REACTANTS     4.71E18       -1.0        0.0        0.0        0.0        0.0  1.0     0
O                       1O   1                 G
H                       1H   1                 G
PRODUCTS
OH                      1O   1H   1            G
EFFICIENCY
       1.0        1.0        1.0        1.0        1.0        1.0        1.0
       1.0        1.0        1.0

;7TH REACTION  CO + O2 <-> CO2 + O
REACTANTS     5.06E13       0.0    31800.0        0.0        0.0        0.0  0.0     0
O2                      1O   2                 G
CO                      1C   1O   1            G
PRODUCTS
CO2                     1C   1O   2            G
O                       1O                     G
KEND
```

Appendix B. Example Input Number 2

This appendix appears in its original form, without editorial change.

```
;;-------------------------------------------------------------------------
;; Example erod.in number 2 July 2, 2001
;;-------------------------------------------------------------------------
; Please use"instructions" pamphlet to ensure correct input deck development
;-------------------------------------------------------------------------
; Ambient Temp (R), Pr (psi), gas vel (in/s)    (FROM XKTC FILE: htemp.out)
;  :    ..............:            :         (CRUMMY UNITS ARE FROM THE 70'S)
;  :    :    ......................:
;  :    :    :

530.0 14.70 0.00

;-------------------------------------------------------------------------
; xchrom (in), tmaxv (ms), xcon, xcham (in),
;  :     .........:         :      :
;  :     :     ..............:      :
;  :     :     :    ................:
;  :     :     :    :
;  :     :     :    :   zmax (in) , nloc , zstart (in), zend (in)
;  :     :     :    :    :     ......:         :          :
;  :     :     :    :    :     :    ............:          :
;  :     :     :    :    :     :    :    ..................:
;  :     :     :    :    :     :    :    :  2-D LP chamber option
;  :     :     :    :    :     :    :    :    :   piston offset for 2-D LP calculation (initial)
;  :     :     :    :    :     :    :    :    :    :   IMC (extra card required at end)
;  :     :     :    :    :     :    :    :    :    :    :   insulate outer B.C.
;  :     :     :    :    :     :    :    :    :    :    :    :   blowby (extra card need placed at end)
;  :     :     :    :    :     :    :    :    :    :    :    :    :           (after IMC card if present)
;  :     :     :    :    :     :    :    :    :    :    :    :    :    :   heat transfer coefficient fudge
factor
;  :     :     :    :    :     :    :    :    :    :    :    :    :    :    :
;  :     :     :    :    :     :    :    :    :    :    :    :    :    :    :

0.010  1.0  0.0  22.0  200.  81 19.0 59.0    0    0    0    0    0   -1. augwlower coef

;  ROUGHNESS DATA  (only if heat transfer coef fudge factor is negative)
;  esmooth (m) smooth deformation limit (Moody chart)
;  :           erough (m) rough deformation limit (Moody chart)
;  :           :
   1.524D-6    5.D-2
```

```
                    ; ESMOOTH = 2.540D-4      ! (m) CHROME THICKNESS - CHIPPED VIRGIN TUBE
; ESMOOTH = 1.5240D-6     ! (m) DRAWN TUBING - CHROMED TUBE VIRGIN
; EROUGH  = 5.0D-2        ! (m) CONDEMNATION CRITERA FOR M256 = 0.5cm therefore erough larger than limit
;
; Barrel Geometry :
; ndtz, zdb (1:ndtz) -- no of axial locations, ndtz locations (in)
; (max = 8)
;
;     1       2       3       4       5       6       7       8

2    0.0    200.0

; dbar (1:ndtz)       -- barrel o.d. at ndtz locations (in)

  10.00  10.00

; dbor (1:ndtz)       -- barrel i.d. at ndtz locations (in)
;     1       2       3       4       5       6       7       8

   4.80  4.80

; Desired Output Locations:
;-------------------------------------------------------------------------------
; nhtz, zout (1:nhtz)-- no of locations for output, nhtz locations (in)
; (max =8)
;    1       2       3       4       5       6       7       8

8  25.    29.     33.     37.     41.     45.     49.     53.

; rout (1:nhtz)       -- radial depth at nhtz locations (in)
;    1       2       3       4       5       6       7       8

 0.010   0.010   0.010   0.010   0.010   0.010   0.010   0.010

; EROSION DATA CARD (BASE MATERIAL!)
;   .... ICHEM  (2) EQUILIBRIUM AND KINETICS ON (1) EQUILIBRIUM ONLY ON (0) OFF
;   :    .... FREEZE-OUT TEMPERATURE (i.e. ICHEM=0) (K)
;   :    :       ..... DENSITY IN (kg/m3)
;   :    :       :       ......MELT TEMP (K)
;   :    :       :       :       .......OUTER BARREL HEAT TRANSFER COEF (W/m2/K)
;   :    :       :       :       :      ..... AMBIENT AIR TEMP (K) (OUTSIDE)
```

```
;  :   :       :       :       :      :      ..... COMPUTATIONAL COORD SPACING (-)
;  :   :       :       :       :      :      :     ..... LATENT HEAT OF FUSION (J/kg)
;  :   :       :       :       :      :      :     :       .... (0) PLANER (1) AXISYMETRIC
;  :   :       :       :       :      :      :     :       :  .... TMIX control volume temperature
;  :   :       :       :       :      :      :     :       :  :      (1)molecular weighting function
;  :   :       :       :       :      :      :     :       :  :         (0)wall temp
;  :   :       :       :       :      :      :     :       :  :
;  :   :       :       :       :      :      :     :       :  :

    2  750.0  7827.0  1720.0  6.0  298.0  1.0  2.7E+5  1  0

; EROSION COATING DATA CARD ONLY IF CHROME GT 0.D0
;    ...NUMBER OF RADIAL PTS IN COATING (-)
;    :      .....NUMBER OF RADIAL PTS IN BASE MATERIAL (-)
;    :      :      .... FREEZE-OUT TEMPERATURE (i.e. ICHEM=0) (K)
;    :      :      :       .....  DENSITY IN (kg/m3)
;    :      :      :       :       ......MELT TEMP (K)
;    :      :      :       :       :      ..... COMPUTATIONAL COORD SPACING (-)
;    :      :      :       :       :      :     .... LATENT HEAT OF FUSION (J/kg)
;    :      :      :       :       :      :     :       ...COATING STRESS FLAG (-)
;    :      :      :       :       :      :     :       :
;    :      :      :       :       :      :     :       :
;    :      :      :       :       :      :     :       :
;    :      :      :       :       :      :     :       :
;

   35    65    250.0  16650.0 3269.  1.0  1.7E+5   1      Ta
;   35    65    250.0  7827.0  2133.0  1.0  2.7E+5  1     chrome

;  COATING STRESS CALCULATION CARD - ONLY IF COATING STRESS FLAG GT 0
;       .... Youngs Modulus Coating (Pa)
;       :       .... CTE Coating (1/K)
;       :       :       .... Poisson's Ratio Coating (-)
;       :       :       :       .... Ultimate Strength Coating (Pa)
;       :       :       :       :       .... Youngs Modulus Base (Pa)
;       :       :       :       :       :       .... CTE Base(1/K)
;       :       :       :       :       :       :       .... Poisson's Ratio Base (-)
;       :       :       :       :       :       :       :

    186.D9  6.8D-6  0.35D0  900.D6  211.D9 12.6D-6  .296D0
;     TA      TA      TA      TA     4340    4340    4340
```

```
;   248.D9  6.5D-6  0.21D0  413.D6  211.D9 12.6D-6  .296D0
;  chrome  chrome  chrome   chrome   4340    4340    4340
;  chrome data from www.matweb.com
;  4340 data from 4340 material data sheet

;  CRACK CALCULATION CARD - ONLY IF COATING STRESS FLAG GT 0
;     ....  Crack Width (m)
;     :       ....  Crack Distribution Limit (m) for augmentation of HXF in crack
;     :       :

  2.D-4     50.0

;  crack width - estimated
;  crack distribution limit - estimated

; Firing Data:
;-------------------------------------------------------------------------------
; nrounds, nkount1, nkount2, deltv (s), lastshot
;   ..........:       :            :       :
;   :    ............:            :       :
;   :    :      ...................:       :
;   :    :      :    ......................:
;   :    :      :    :

1   5   20   10D-6   0

; Desired Output Units and Files:
;-------------------------------------------------------------------------------
;
; iunit (0 for K, 1 for deg R)
;   ___ itemp (0 for as calculated, 1 for temp rise),
; |
; |  _______. screen output                          (single shot-1, burst-2)        IOUT(1)
; | |                                    iout (1:9) ---
; | |  _______ single shot probe temperature,                                      IOUT(2)
; | | |_______single shot inside surface temperature,                              IOUT(3)
; | | | _______single shot outside surface temperature,                            IOUT(4)
; | | | |
; | | | |  _____ burst fire probe temperature,                                     IOUT(5)
; | | | | |____ burst fire inside surface temperature,                             IOUT(6)
; | | | | | ___ burst fire outside surface temperature,                            IOUT(7)
```

```
;  | | | | | | | |
;  | | | | | | | |  ___ heat transfer coefficient,                                  IOUT(8)
;  | | | | | | | |  |  ___ effective gas temperature history                        IOUT(9)
;  | | | | | | | |  |  |
;  | | | | | | | |  |  |  ___ single shot graphics output (for IBGRAF)              IOUT(10)
;  | | | | | | | |  |  |  |  ___  burst fire graphics output (for IBGRAF)       IOUT(11)
;  | | | | | | | |  |  |  |  |  ___ boundary condition graphic output (for IBGRAF)  IOUT(12)
;  | | | | | | | |  |  |  |  |  |
;  | | | | | | | |  |  |  |  |  |  ___ bore surface heat flux output              IOUT(13)
;  | | | | | | | |  |  |  |  |  |  |  ___ bore surface regression rate            IOUT(14)
;  | | | | | | | |  |  |  |  |  |  |  |  ___ bore surface regression              IOUT(15)
;  | | | | | | | |  |  |  |  |  |  |  |  |  __ core species concentration (-)     IOUT(16)
;  | | | | | | | |  |  |  |  |  |  |  |  |  |  __ wall species concentrations(-)  IOUT(17)
;  | | | | | | | |  |  |  |  |  |  |  |  |  |  |  __ interfacial shear (MPa)      IOUT(18)
;  | | | | | | | |  |  |  |  |  |  |  |  |  |  |  |  __ interfacial axial shear (MPa) IOUT(19)
;  | | | | | | | |  |  |  |  |  |  |  |  |  |  |  |  |  __ blank                   IOUT(20)
;  | | | | | | | |  |  |  |  |  |  |  |  |  |  |  |  |  |

0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0

;  Variable   Property: k Barrel    Alpha Barrel      k Liner    Alpha Liner
;  Property   Material:   (4340)          (4340)        (TA)          (TA)
;  For 4340   Units:     (W/m/K)         (m2/s)      (W/m/K)       (m2/s)
; (1=y,2=no)  Source:     [TPOM]          [TPOM]        [I&D]         [I&D]
      1                    34.1          9.6e-6         60.2     2.3397e-5

; Note: The variable property option overrides the other property inputs Alpa,Cp
; New physical property inputs are in units of W,m,s,K (only for version v32 and above)

; 304SS k  pg. 1164 curve 11 TPOM Vol. 1   0.180  W/cm/K @523K  = 18.0 W/m/K
; 304SS k  pg. 1164 curve 11 TPOM Vol. 1   0.219  W/cm/K @823K  = 21.9 W/m/K
; 4340  k  pg. 1212 curve 21 TPOM Vol. 1   0.335  W/cm/K @295K  = 33.5 W/m/K
; 4340  k  pg. 1212 curve 25 TPOM Vol. 1   0.341  W/cm/K @813K  = 34.1 W/m/K
; CHROME k pg. 755  Inc. and Dewitt        0.807  W/cm/K @ 600K = 80.7 W/m/K
; CHROME k pg. 755  Inc. and Dewitt        0.654  W/cm/K @1000K = 65.4 W/m/K
; Comp. k11 = k22 Tzeng Comp. Man. V4 #3   0.0071 W/cm/K        = 0.71 W/m/K
; Comp. k33 Tzeng       Comp. Man. V4 #3   0.160  W/cm/K        = 16.0 W/m/K
; 304SS   g. 344  curve 11 TPOM Vol.10   0.0352 cm2/s @ 460K  = 3.52e-6 m2/s
; 304SS   g. 344  curve 11 TPOM Vol.10   0.0457 cm2/s @1146K  = 4.57e-6 m2/s
; 4340    g. 362  curve 2  TPOM Vol.10   0.096  cm2/s @ 313K  = 9.6e-6  m2/s
; 4340    g. 362  curve 3  TPOM Vol.10   0.087  cm2/s @ 313K  = 8.7e-6  m2/s
```

```
; 4340    g. 362  curve 3  TPRC Vol.10   0.057  cm2/s @1203K  = 5.7e-6  m2/s
; CHROME  . 755  Inc. and Dewitt         0.207  cm2/s @ 600K  = 2.0795e-5m2/s
; CHROME  . 755  Inc. and Dewitt         0.148  cm2/s @1000K  = 1.4828e-5m2/s
; Composite Tzeng Comp. Manu. Vol 4 no 3   0.0051 cm2/s         = 5.10e-7 m2/s
; Composite Tzeng Comp. Manu. Vol 4 no 3   0.1150 cm2/s         = 1.15e-5 m2/s

42
This species input section is keyed on key phrases in the following notes:
Also the previous number "42" is a "magic number" flag
1.SPECIES NAME MUST MATCH NASA LEWIS LIBRARY NAME EXACTLY
2.LEFT JUSTIFIED ELEMENT CHARACTERS
3.RIGHT JUSTIFIED ELEMENT NUMBERS
4.FORMAT (5A4,4(A2,F3.0),A1)
5.LEAVE EXTRAINIOUS FORMAT SEGMENTS BLANK
6.PHASE MUST BE EXPLICITLY SPECIFIED
7.REACTANT ORDER MUST BE THE SAME AS THAT EXTRACTED FROM IB CODE
8.KEY POINTER PHRASES ARE:
FORMAT(A30,I3):                    "NUMBER OF REACTANT ELEMENTS = ",#
CONSIDERED ELEMENTS IN "A" ORDER: "CONSIDERED ELEMENTS = "
BEGINING OF ALL REACTANT CARDS:   "REACTANTS"
BEGINING OF THE PRODUCT CARDS:    "PRODUCTS"

NUMBER OF REACTANT ELEMENTS =
8
CONSIDERED ELEMENTS =
H   C   N   O   S   CR  FE  NI
REACTANTS
;       FORMAT (5A4,4(A2,F3.0),A1,4E10.4)
;FORMULA            ELEMENTS,#      PHASE PCRIT(Pa)  TCRIT(K)  SIGMA(A) EPSOK(K)
;A4][A4][A4][A4][A4][][ ][][ ][][ ][][ ]A[ E10.4  ][  E10.4 ][ E10.4  ][ E10.4 ]
H2                  H   2               G     1.3E6      33.1     2.827   59.7
O2                  O   2               G    5.08E6     154.6     3.467  106.7
CO                  C   10   1          G     3.5E6     133.0     3.690   91.7
CO2                 C   10   2          G    7.39E6     304.0     3.941  195.2
H2O                 H   20   1          G   22.09E6     647.1     2.641  809.1
SO2                 S   10   2          G    7.88E6     430.8     4.112  335.4
N2                  N   2               G    3.39E6     126.0     3.798   71.4
NO                  N   10   1          G    6.48E6     180.0     3.492  116.7
; note: the 1RST solid reactant (9th reactant) must be C(GR) solid phase
C(GR)               C   1               S       1.0       1.0       1.0    1.0
```

```
; note: the 10th reactant must be FE(A) solid phase
FE(A)                FE  1                S       1.0       1.0       1.0    1.0 10
; note: the 11th reactant must be FE(C) solid phase
FE(C)                FE  1                S       1.0       1.0       1.0    1.0 11
NI(B)                NI  1                S       1.0       1.0       1.0    1.0 12
S                    S   1                G       1.0       1.0       1.0    1.0 13
CR2O3(S)             CR  2O   3           S       1.0       1.0       1.0    1.0 14
PRODUCTS
; note: FE3C must be the 15th (reactant+product) to match index in program
FE3C                 FE  3C   1           S       1.0       1.0       1.0     1.0    15
FEO(S)               FE  1O   1           S       1.0       1.0       1.0     1.0    16
FE3O4(S)             FE  3O   4           S       1.0       1.0       1.0     1.0    17
FE2O3(S)             FE  2O   3           S       1.0       1.0       1.0     1.0    18
FEO(L)               FE  1O   1           L       1.0       1.0       1.0     1.0    19
FE                   FE  1                G       1.0       1.0       1.0     1.0    20
FE(L)                FE  1                L       1.0       1.0       1.0     1.0    21
FEO                  FE  1O   1           G       1.0       1.0       1.0     1.0    22
FEO2H2               FE  1O   2H   2      G       1.0       1.0       1.0     1.0    23
H                    H   1                G       1.0       1.0       1.0     1.0    24
O                    O   1                G       1.0       1.0       1.0     1.0    25
; Note:  Neither the critical values nor the Leonard Jones values for O and H in
;        substrate.  This influences neither the surface state nor tranport calculation
NO2                  N   1O   2           G       1.0       1.0       1.0     1.0    26
NI(L)                NI  1                L       1.0       1.0       1.0     1.0    27
OH                   O   1H   1           G       1.0       1.0       1.0     1.0    28
;S2                   S   2                G       1.0       1.0       1.0     1.0    25 -
;COS                  C   1O   1S   1      G       1.0       1.0       1.0     1.0    26 -
;SO                   S   1O   1           G       1.0       1.0       1.0     1.0    27 -
;CRO                  CR  1O   1           G       1.0       1.0       1.0     1.0    28 -
;CRO2                 CR  1O   2           G       1.0       1.0       1.0     1.0    29 -
;HCO RAD              H   1C   1O   1      G       1.0       1.0       1.0     1.0    30 -
;HCN                  H   1C   1N   1      G       1.0       1.0       1.0     1.0    31 -
;HNO                  H   1N   1O   1      G       1.0       1.0       1.0     1.0    32 -
;OH+                  O   1H   1E -1.      G       1.0       1.0       1.0     1.0    15 -
;NIO2H2               NI  1O   2H   2      G       1.0       1.0       1.0     1.0    35 -
;NI                   NI  1                G       1.0       1.0       1.0     1.0    36 -
;NIO                  NI  1O   1           G       1.0       1.0       1.0     1.0    37 -
EQEND
;   SIGMA, EPSOK,   SOURCE   - MARTIN MILLER'S BOOK AND HIRSHFIELDER
;   TCRIT, PCRIT,   SOURCE   - VAN WEHLAN AND SONNTAG
```

```
KINETICS BEGIN REACTION CARDS
;  ..NUMBER OF KINETIC REACTANT SPECIES
;  :    ..NUMBER OF REACTIONS
;  :    :
  10    7
;        FORMAT(4(5A4))

CO2                  CO                   O2                   C(GR)
FE(A)                O                    H2O                  H2
H                    OH

CONSIDERED SPECIES FOR KINETIC REACTIONS
;         .. REACTANTS "KEY WORD" FORMAT(A10,7E10.4,I5)
;         :          ..  CF (CM3/MOLE-S) or (CM6/MOLE2-S) FORWARD RATES
;         :          :         ..ETAF (-)
;         :          :         :          .. EF/k (K) (0 => NOT CONSIDERED, -1 => COMPUTED)
;         :          :         :          :     (cal -> need icofu=1)
;         :          :         :          :          .. CB (CM3/MOLE-S) or (CM6/MOLE2-S) REV RATES
;         :          :         :          :          :          .. ETAB (-)
;         :          :         :          :          :          :          .. EB/k(K)(0=>NOT,-1=>THERMO)
;         :          :         :          :          :          :          :    .. THIRDBODY (-)
;         :          :         :          :          :          :          :    :    (1=T, 0=F)
;         :          :         :          :          :          :          :    :    ..ICOFU (-)
;         :          :         :          :          :          :          :    :    :  (0 NORMAL 1 = SURFACE)
;         :          :         :          :          :          :          :    :    :
;1RST REACTION    CO + O <-> CO2    3rd order rxn
REACTANTS    6.17E14       0.0    1510.0       0.0       0.0       0.0  1.0    0
;   FORMAT (5A4,F3.0,4(A2,F3.0),A1,4E10.4)
CO                       1C   1O   1          G
O                        1O   1               G
PRODUCTS
CO2                      1C   1O   2          G
EFFICIENCY
       1.0       1.0       1.0       1.0       1.0       1.0       1.0
       1.0       1.0       1.0

;2ND REACTION  CO + Fe <-> Fe + C + O
REACTANTS     5.2E14       0.0   23903.0       0.0       0.0       0.0  0.0    0
CO                       1C   1O   1          G
FE(A)                    1FE  1               S
PRODUCTS
```

```
O                       1O   1                 G
C(GR)                   1C   1                 S
FE(A)                   1FE  1                 S
;note: if NOT 3rd body RXN, KEND is required
KEND

;3RD REACTION     O + O <-> O2
REACTANTS    1.89E13          0.0     -900.0        0.0        0.0        0.0  1.0     0
O                       2O   1                 G
PRODUCTS
O2                      1O   2                 G
EFFICIENCY
       1.0        1.0         1.0         1.0        1.0        1.0        1.0
       1.0        1.0         1.0

;4RTH REACTION  H + OH <-> H2O
REACTANTS    8.35E21         -2.0         0.0        0.0        0.0        0.0  1.0     0
OH                      1O   1H   1            G
H                       1H   1                 G
PRODUCTS
H2O                     1H   2O   1            G
EFFICIENCY
       1.0        1.0         1.0         1.0        1.0        1.0        1.0
       1.0        1.0         1.0

;5TH REACTION  H2 + FE <-> H + H + FE
REACTANTS    4.57E19         -1.4    52530.0        0.0        0.0        0.0  0.0     0
H2                      1H   2                 G
FE(A)                   1FE  1                 S
PRODUCTS
FE(A)                   1FE  1                 S
H                       2H   1                 G
KEND

;6TH REACTION  H + O <-> OH
REACTANTS    4.71E18         -1.0         0.0        0.0        0.0        0.0  1.0     0
O                       1O   1                 G
H                       1H   1                 G
PRODUCTS
OH                      1O   1H   1            G
EFFICIENCY
```

```
      1.0       1.0       1.0       1.0       1.0       1.0       1.0
      1.0       1.0       1.0

;7TH REACTION  CO + O2 <-> CO2 + O
REACTANTS    5.06E13        0.0    31800.0        0.0       0.0       0.0  0.0    0
O2                     1O    2                 G
CO                     1C    1O    1           G
PRODUCTS
CO2                    1C    1O    2           G
O                      1O                      G
KEND
```

Appendix C. Example of "species.out" File

This appendix appears in its original form, without editorial change.

-Time_(ms),	------N2-,	------CO-,	-----H2O-,	------H2-,	-----CO2-,	-----KOH-,	------NO-,	-----COS-,	------O2-,	-----NH3-,
0.0000,	2.773E-01,	2.740E-01,	2.498E-01,	1.200E-01,	6.843E-02,	2.115E-03,	3.748E-04,	9.378E-05,	4.045E-05,	2.475E-05,
0.0500,	2.820E-01,	2.741E-01,	2.429E-01,	1.261E-01,	6.511E-02,	1.947E-03,	3.321E-04,	9.704E-05,	3.205E-05,	2.880E-05,
0.1000,	2.884E-01,	2.715E-01,	2.372E-01,	1.311E-01,	6.245E-02,	1.810E-03,	3.000E-04,	9.926E-05,	3.272E-05,	2.635E-05,
0.1500,	2.886E-01,	2.714E-01,	2.372E-01,	1.309E-01,	6.218E-02,	1.815E-03,	3.268E-04,	9.745E-05,	3.432E-05,	2.937E-05,
0.2000,	2.962E-01,	2.683E-01,	2.303E-01,	1.371E-01,	5.912E-02,	1.653E-03,	2.854E-04,	9.995E-05,	4.025E-05,	2.273E-05,
0.2500,	3.028E-01,	2.655E-01,	2.240E-01,	1.428E-01,	5.656E-02,	1.508E-03,	2.438E-04,	1.019E-04,	4.559E-05,	1.723E-05,
0.3000,	3.088E-01,	2.630E-01,	2.183E-01,	1.479E-01,	5.422E-02,	1.382E-03,	2.179E-04,	1.025E-04,	5.244E-05,	2.249E-05,
0.3500,	3.140E-01,	2.608E-01,	2.131E-01,	1.526E-01,	5.224E-02,	1.267E-03,	1.911E-04,	1.027E-04,	5.844E-05,	2.596E-05,
0.4000,	3.187E-01,	2.587E-01,	2.084E-01,	1.568E-01,	5.041E-02,	1.166E-03,	1.738E-04,	1.020E-04,	6.630E-05,	3.063E-05,
0.4500,	3.189E-01,	2.587E-01,	2.085E-01,	1.567E-01,	5.026E-02,	1.170E-03,	1.819E-04,	1.021E-04,	6.961E-05,	3.257E-05,
0.5000,	3.231E-01,	2.569E-01,	2.043E-01,	1.605E-01,	4.865E-02,	1.079E-03,	1.653E-04,	1.012E-04,	7.853E-05,	3.805E-05,
0.5500,	3.269E-01,	2.552E-01,	2.004E-01,	1.641E-01,	4.727E-02,	9.956E-04,	1.487E-04,	9.975E-05,	8.603E-05,	4.282E-05,
0.6000,	3.303E-01,	2.537E-01,	1.968E-01,	1.673E-01,	4.598E-02,	9.217E-04,	1.369E-04,	9.820E-05,	9.618E-05,	4.934E-05,
0.6500,	3.334E-01,	2.524E-01,	1.936E-01,	1.702E-01,	4.487E-02,	8.532E-04,	1.250E-04,	1.045E-04,	9.606E-05,	5.488E-05,
0.7000,	3.362E-01,	2.511E-01,	1.907E-01,	1.729E-01,	4.382E-02,	7.924E-04,	1.162E-04,	1.160E-04,	9.410E-05,	6.254E-05,
0.7500,	3.372E-01,	2.507E-01,	1.898E-01,	1.736E-01,	4.344E-02,	7.749E-04,	1.230E-04,	1.147E-04,	9.389E-05,	6.716E-05,
0.8000,	3.389E-01,	2.500E-01,	1.881E-01,	1.752E-01,	4.277E-02,	7.399E-04,	1.349E-04,	1.104E-04,	9.304E-05,	7.511E-05,
0.8500,	3.412E-01,	2.490E-01,	1.856E-01,	1.774E-01,	4.195E-02,	6.877E-04,	1.453E-04,	1.022E-04,	9.041E-05,	8.241E-05,
0.9000,	3.433E-01,	2.480E-01,	1.834E-01,	1.795E-01,	4.116E-02,	6.413E-04,	1.600E-04,	9.576E-05,	9.271E-05,	8.825E-05,
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1.0001,	3.471E-01,	2.463E-01,	1.831E-01,	1.794E-01,	3.982E-02,	5.583E-04,	1.884E-04,	1.130E-04,	8.431E-05,	8.325E-05,
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1.1501,	3.503E-01,	2.449E-01,	1.860E-01,	1.761E-01,	3.862E-02,	4.899E-04,	2.314E-04,	1.442E-04,	7.941E-05,	7.536E-05,
1.2001,	3.517E-01,	2.443E-01,	1.873E-01,	1.747E-01,	3.810E-02,	4.590E-04,	2.529E-04,	1.601E-04,	7.722E-05,	7.131E-05,
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14. ABSTRACT
This report documents the U.S. Army Research Laboratory Gun Tube Erosion Code (ATEC) user input as well as output from the code. Instructions for developing an input deck are explicitly provided to assist the user. Each input variable is described, and units are provided where necessary. The appendices include examples of various input decks and an example of the species input file. Files required to operate the code include a user-generated input deck, an output file HTEMP.OUT from XKTC (Gough, P. S. "The XNOVAKTC Code." BRL-CR-627, U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, 1990), the NASA Lewis library (Gordon, S., and B. J. McBride. "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouget Detonations." NASA SP-273, NASA Lewis, Cleveland, OH, 1971), and a species temporal file, "species.out", from a coupled interballistic equilibrium thermodynamic code. The ATEC code has been applied to the 25-mm Bushmaster cannon, Navy 5-in cannons, the 120-mm M256 tank cannon, as well as various vented fixtures, and has performed well in representing the physics which occurs at the surface.

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gun tube erosion, surface chemistry

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